



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:01 AM UTC

PDB ID : 6COF / pdb_00006cof
Title : AtHNL enantioselectivity mutant At-A9-H7 Apo, Y13C,Y121L,P126F,L128
W,C131T,A209I
Authors : Jones, B.J.; Kazlauskas, R.J.; Desrouleaux, R.
Deposited on : 2018-03-12
Resolution : 1.52 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

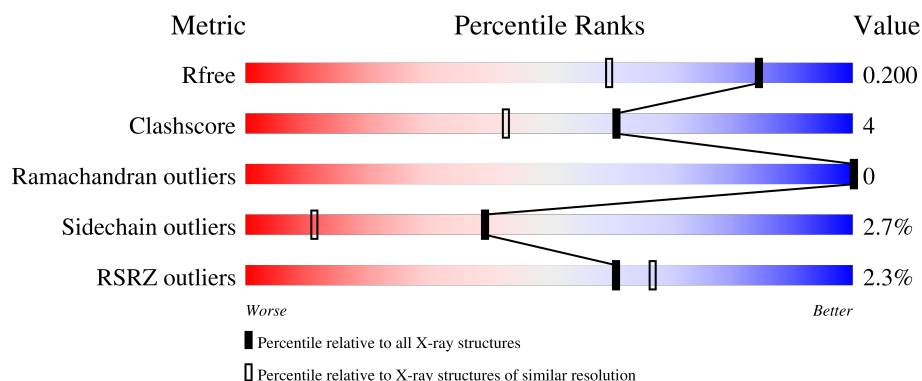
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.52 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5890 (1.54-1.50)
Clashscore	190562	6116 (1.54-1.50)
Ramachandran outliers	187476	6002 (1.54-1.50)
Sidechain outliers	187428	5999 (1.54-1.50)
RSRZ outliers	180081	5891 (1.54-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	260	2% 67% 27% 5%
1	B	260	2% 75% 22% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4587 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Alpha-hydroxynitrile lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	5	0
			2103	1353	348	386	16			
1	B	259	Total	C	N	O	S	0	7	0
			2111	1358	345	391	17			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	CYS	TYR	engineered mutation	UNP Q9LFT6
A	122	LEU	TYR	engineered mutation	UNP Q9LFT6
A	126	PHE	PRO	engineered mutation	UNP Q9LFT6
A	129	TRP	LEU	engineered mutation	UNP Q9LFT6
A	132	THR	CYS	engineered mutation	UNP Q9LFT6
A	210	ILE	ALA	engineered mutation	UNP Q9LFT6
A	259	GLY	-	expression tag	UNP Q9LFT6
A	260	LEU	-	expression tag	UNP Q9LFT6
B	14	CYS	TYR	engineered mutation	UNP Q9LFT6
B	122	LEU	TYR	engineered mutation	UNP Q9LFT6
B	126	PHE	PRO	engineered mutation	UNP Q9LFT6
B	129	TRP	LEU	engineered mutation	UNP Q9LFT6
B	132	THR	CYS	engineered mutation	UNP Q9LFT6
B	210	ILE	ALA	engineered mutation	UNP Q9LFT6
B	259	GLY	-	expression tag	UNP Q9LFT6
B	260	LEU	-	expression tag	UNP Q9LFT6

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		

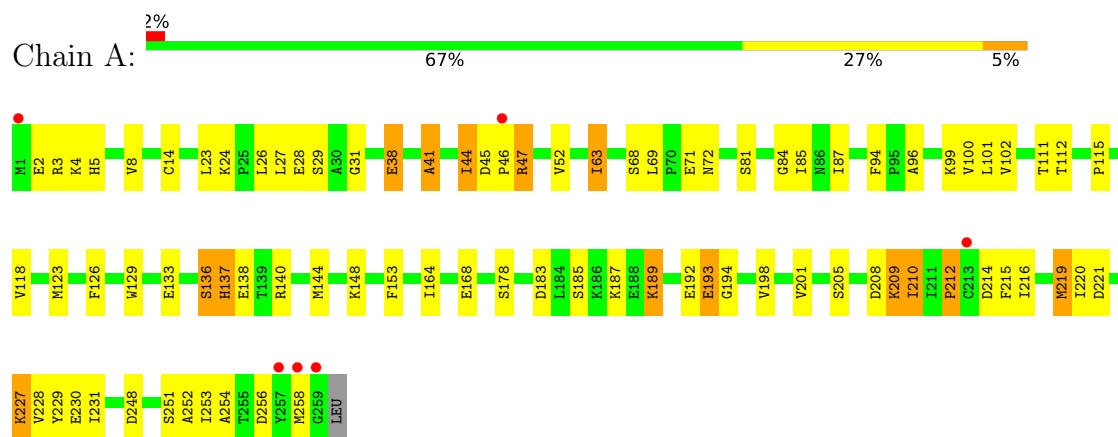
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	171	Total	O	0	0
			171	171		
4	B	188	Total	O	0	0
			188	188		

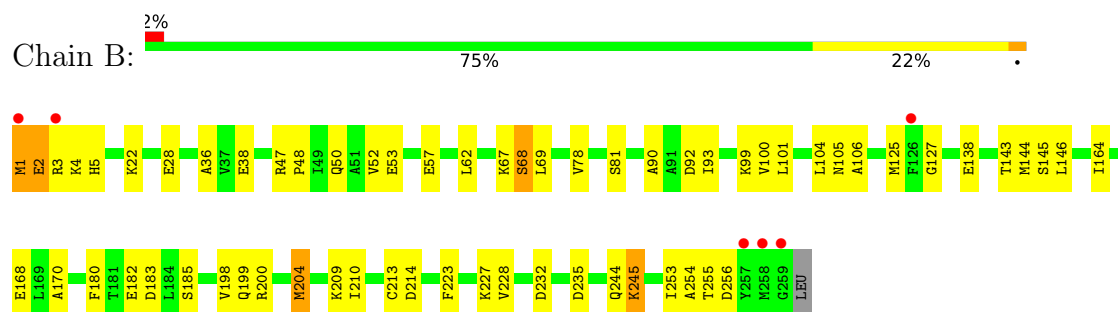
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Alpha-hydroxynitrile lyase



• Molecule 1: Alpha-hydroxynitrile lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.84Å 87.09Å 123.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.52 50.00 – 1.52	Depositor EDS
% Data completeness (in resolution range)	98.9 (50.00-1.52) 98.9 (50.00-1.52)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 1.52Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.158 , 0.191 0.171 , 0.200	Depositor DCC
R_{free} test set	4180 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4587	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.14	72/2161 (3.3%)	1.77	30/2917 (1.0%)
1	B	2.03	47/2169 (2.2%)	1.66	26/2927 (0.9%)
All	All	2.08	119/4330 (2.7%)	1.71	56/5844 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (119) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	81	SER	CA-C	12.07	1.64	1.52
1	B	210	ILE	CA-CB	10.91	1.66	1.55
1	A	81	SER	CA-C	10.22	1.62	1.52
1	A	47[A]	ARG	CA-C	9.57	1.63	1.53
1	A	47[B]	ARG	CA-C	9.57	1.63	1.53
1	A	52	VAL	C-N	-8.79	1.20	1.33
1	B	256	ASP	N-CA	8.18	1.57	1.46
1	B	48	PRO	N-CA	-8.00	1.38	1.46
1	A	111	THR	CA-C	7.99	1.63	1.52
1	B	144	MET	SD-CE	-7.78	1.60	1.79
1	A	26	LEU	C-O	7.56	1.32	1.24
1	A	23	LEU	C-O	7.55	1.33	1.24
1	B	253	ILE	CA-CB	7.54	1.63	1.54
1	B	2	GLU	CA-C	7.45	1.61	1.52
1	A	212	PRO	CA-C	-7.39	1.43	1.52
1	B	93	ILE	C-O	7.38	1.31	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	140	ARG	CA-C	7.15	1.62	1.52
1	A	45	ASP	C-O	7.14	1.32	1.24
1	A	99	LYS	N-CA	7.08	1.55	1.46
1	A	129	TRP	N-CA	7.05	1.55	1.46
1	A	44	ILE	C-O	7.02	1.32	1.24
1	B	47	ARG	CZ-NH1	6.87	1.42	1.32
1	A	178	SER	CA-C	-6.84	1.43	1.52
1	B	210	ILE	CB-CG1	-6.83	1.39	1.53
1	A	214	ASP	C-O	-6.82	1.16	1.24
1	B	255	THR	N-CA	6.78	1.54	1.46
1	A	231	ILE	C-O	6.76	1.31	1.24
1	B	81	SER	C-O	6.75	1.31	1.24
1	A	123	MET	N-CA	-6.55	1.38	1.46
1	B	22	LYS	CD-CE	-6.52	1.32	1.52
1	A	26	LEU	N-CA	6.47	1.54	1.46
1	A	94	PHE	CA-CB	6.45	1.60	1.53
1	B	204	MET	CA-C	-6.45	1.44	1.52
1	A	251	SER	N-CA	6.42	1.54	1.46
1	A	101	LEU	CA-CB	-6.41	1.44	1.53
1	A	4	LYS	N-CA	6.39	1.53	1.45
1	B	67	LYS	N-CA	6.39	1.54	1.46
1	A	219	MET	C-O	-6.38	1.16	1.24
1	B	185	SER	N-CA	6.38	1.54	1.46
1	B	180	PHE	CA-C	6.38	1.61	1.53
1	A	194	GLY	CA-C	-6.35	1.48	1.51
1	A	14	CYS	CA-CB	-6.34	1.45	1.54
1	A	205	SER	N-CA	-6.31	1.37	1.46
1	A	227	LYS	N-CA	-6.26	1.38	1.46
1	A	41	ALA	CA-C	-6.26	1.44	1.53
1	A	26	LEU	CA-CB	-6.25	1.43	1.53
1	A	168	GLU	CD-OE2	6.23	1.37	1.25
1	A	123	MET	SD-CE	-6.21	1.64	1.79
1	A	148	LYS	CA-C	-6.20	1.45	1.52
1	B	68	SER	CA-C	6.08	1.61	1.52
1	A	29	SER	N-CA	6.06	1.54	1.46
1	A	137	HIS	N-CA	-6.06	1.38	1.46
1	A	136	SER	CB-OG	-6.03	1.30	1.42
1	A	102	VAL	CA-CB	-6.03	1.46	1.53
1	A	27	LEU	C-O	6.02	1.31	1.24
1	B	36	ALA	CA-C	5.98	1.60	1.53
1	A	94	PHE	N-CA	-5.96	1.40	1.46
1	A	46	PRO	C-O	5.94	1.31	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	143	THR	CA-CB	-5.94	1.44	1.53
1	B	254	ALA	CA-CB	-5.92	1.44	1.53
1	B	50	GLN	C-O	5.91	1.31	1.24
1	B	90	ALA	C-O	5.90	1.31	1.24
1	A	187	LYS	N-CA	-5.90	1.38	1.45
1	A	228	VAL	CA-C	-5.88	1.45	1.52
1	B	182	GLU	C-O	5.88	1.30	1.24
1	A	101	LEU	N-CA	5.87	1.53	1.46
1	A	185	SER	N-CA	5.85	1.53	1.46
1	A	28	GLU	N-CA	5.84	1.53	1.46
1	B	101	LEU	C-O	5.83	1.31	1.23
1	B	223	PHE	CA-C	-5.82	1.48	1.53
1	A	148	LYS	C-O	5.81	1.30	1.24
1	B	47	ARG	NE-CZ	-5.79	1.26	1.33
1	B	255	THR	CA-CB	-5.79	1.44	1.53
1	A	69	LEU	C-O	-5.75	1.16	1.24
1	B	78	VAL	CA-CB	-5.73	1.47	1.54
1	A	126	PHE	C-O	5.69	1.30	1.24
1	A	248	ASP	N-CA	5.68	1.53	1.46
1	B	199	GLN	N-CA	-5.68	1.39	1.46
1	A	221	ASP	CB-CG	-5.66	1.37	1.52
1	A	144	MET	C-O	-5.64	1.17	1.24
1	B	146	LEU	C-O	5.63	1.30	1.23
1	B	232	ASP	N-CA	-5.55	1.39	1.46
1	B	168	GLU	CD-OE2	5.53	1.35	1.25
1	B	182	GLU	CD-OE1	5.51	1.35	1.25
1	A	99	LYS	C-O	-5.50	1.17	1.24
1	B	106	ALA	N-CA	-5.48	1.39	1.45
1	A	8	VAL	CA-CB	-5.47	1.47	1.54
1	B	183	ASP	N-CA	-5.44	1.39	1.46
1	B	198	VAL	N-CA	-5.39	1.39	1.46
1	B	228	VAL	CA-C	-5.38	1.46	1.52
1	A	44	ILE	CA-C	5.37	1.60	1.52
1	A	45	ASP	C-N	5.36	1.40	1.34
1	A	137	HIS	CA-CB	5.35	1.63	1.53
1	A	153	PHE	C-O	-5.33	1.18	1.24
1	A	198	VAL	CA-CB	5.32	1.61	1.54
1	B	255	THR	C-O	5.32	1.30	1.24
1	A	216	ILE	N-CA	5.32	1.52	1.46
1	B	67	LYS	C-O	5.29	1.30	1.24
1	A	118	VAL	CA-CB	5.27	1.61	1.54
1	A	136	SER	N-CA	5.26	1.52	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	201	VAL	N-CA	-5.26	1.40	1.46
1	A	220	ILE	N-CA	5.25	1.52	1.46
1	A	251	SER	CA-CB	-5.21	1.45	1.53
1	B	28	GLU	C-O	5.20	1.30	1.24
1	A	138	GLU	C-O	5.20	1.30	1.24
1	B	3	ARG	CA-C	5.19	1.59	1.52
1	A	24	LYS	C-N	-5.18	1.27	1.33
1	B	198	VAL	CA-CB	5.17	1.61	1.54
1	B	227	LYS	C-O	5.17	1.30	1.23
1	A	253	ILE	N-CA	-5.14	1.40	1.46
1	B	36	ALA	CA-CB	-5.12	1.46	1.53
1	A	72	ASN	CA-CB	5.12	1.60	1.53
1	A	183	ASP	CA-C	-5.12	1.46	1.52
1	A	230	GLU	CA-C	-5.12	1.46	1.52
1	A	252	ALA	N-CA	5.09	1.52	1.46
1	B	256	ASP	CB-CG	-5.08	1.39	1.52
1	B	53	GLU	CD-OE2	-5.08	1.15	1.25
1	A	23	LEU	CA-CB	-5.07	1.45	1.53
1	A	208	ASP	C-O	5.01	1.29	1.24

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	ASP	CA-C-O	14.29	133.89	120.02
1	B	256	ASP	N-CA-C	10.07	124.95	112.87
1	A	210	ILE	CB-CA-C	9.06	120.00	111.30
1	B	127	GLY	CA-C-N	-7.96	113.01	121.45
1	B	127	GLY	C-N-CA	-7.96	113.01	121.45
1	B	144	MET	CG-SD-CE	-7.65	84.07	100.90
1	A	136	SER	CB-CA-C	-7.51	95.09	109.66
1	A	52	VAL	CB-CA-C	-7.08	102.33	111.53
1	A	8	VAL	N-CA-C	-7.05	97.57	107.80
1	B	214	ASP	N-CA-C	6.76	118.65	111.28
1	B	100	VAL	CA-C-O	-6.14	115.19	120.96
1	B	209	LYS	CA-C-N	6.14	129.93	122.63
1	B	209	LYS	C-N-CA	6.14	129.93	122.63
1	A	96	ALA	N-CA-C	6.08	119.96	112.54
1	B	62	LEU	O-C-N	6.06	128.63	122.09
1	B	210	ILE	CB-CA-C	-6.03	104.69	111.80
1	B	100	VAL	O-C-N	5.97	128.92	123.19
1	A	85	ILE	O-C-N	-5.89	116.14	121.91
1	A	45	ASP	CA-C-N	-5.86	113.92	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	ASP	C-N-CA	-5.86	113.92	119.84
1	A	100	VAL	O-C-N	5.84	128.79	123.19
1	A	84	GLY	O-C-N	-5.80	116.63	122.19
1	B	125	MET	N-CA-CB	-5.80	102.35	111.39
1	A	210	ILE	CA-CB-CG1	5.75	120.18	110.40
1	B	235	ASP	CA-CB-CG	5.74	118.34	112.60
1	B	255	THR	N-CA-C	-5.73	104.93	111.07
1	A	256	ASP	N-CA-C	5.67	119.45	112.54
1	B	228	VAL	O-C-N	-5.64	117.16	123.26
1	A	87	ILE	CA-C-O	-5.64	114.38	120.47
1	B	38	GLU	OE1-CD-OE2	5.57	136.26	122.90
1	A	254	ALA	N-CA-C	-5.56	105.30	111.36
1	A	216	ILE	CA-C-O	5.51	126.68	120.95
1	B	69	LEU	O-C-N	5.47	127.55	121.43
1	A	47[A]	ARG	CA-C-O	5.46	126.27	120.64
1	A	47[B]	ARG	CA-C-O	5.46	126.27	120.64
1	A	31	GLY	CA-C-O	5.43	125.04	119.01
1	A	214	ASP	CB-CA-C	-5.38	101.70	110.85
1	B	145	SER	CA-CB-OG	-5.38	100.33	111.10
1	A	209	LYS	CA-C-N	-5.38	117.44	122.66
1	A	209	LYS	C-N-CA	-5.38	117.44	122.66
1	B	52	VAL	CA-C-N	-5.37	112.98	122.26
1	B	52	VAL	C-N-CA	-5.37	112.98	122.26
1	B	254	ALA	CA-C-O	-5.35	114.87	120.55
1	B	68	SER	CA-CB-OG	-5.33	100.44	111.10
1	B	245	LYS	O-C-N	-5.33	116.08	122.15
1	A	63	ILE	CB-CG1-CD1	5.31	124.96	113.80
1	A	187	LYS	CB-CG-CD	-5.29	99.13	111.30
1	A	38	GLU	CG-CD-OE1	-5.28	106.25	118.40
1	B	254	ALA	O-C-N	5.21	127.64	122.12
1	B	170	ALA	CA-C-O	5.17	126.03	120.55
1	A	251	SER	N-CA-C	-5.12	105.78	111.36
1	A	5	HIS	O-C-N	5.11	129.40	122.96
1	A	189	LYS	N-CA-CB	5.04	117.71	109.69
1	B	200	ARG	NE-CZ-NH2	-5.04	114.67	119.20
1	A	46	PRO	N-CA-C	5.03	121.22	114.22
1	A	212	PRO	CB-CA-C	-5.03	104.97	111.46

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	44	ILE	Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2103	0	2088	21	0
1	B	2111	0	2088	14	0
2	A	12	0	16	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	171	0	0	6	0
4	B	188	0	0	6	0
All	All	4587	0	4192	35	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (35) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47[B]:ARG:HH21	1:A:47[B]:ARG:CG	1.14	1.47
1:A:47[B]:ARG:HH21	1:A:47[B]:ARG:CB	1.69	1.06
1:A:47[B]:ARG:HG2	1:A:47[B]:ARG:NH2	1.27	1.05
1:A:209:LYS:NZ	4:A:401:HOH:O	2.00	0.91
1:A:47[B]:ARG:HH21	1:A:47[B]:ARG:HG2	0.77	0.88
1:A:47[B]:ARG:CG	1:A:47[B]:ARG:NH2	1.93	0.88
1:B:138[B]:GLU:HG2	4:B:487:HOH:O	1.74	0.86
1:A:68:SER:OG	4:A:402:HOH:O	2.04	0.74
1:B:57[B]:GLU:OE2	4:B:401:HOH:O	2.07	0.72
1:A:136:SER:HB3	4:A:430:HOH:O	1.91	0.70
1:B:68:SER:OG	4:B:402:HOH:O	2.10	0.70
1:A:47[B]:ARG:NH2	1:A:47[B]:ARG:HB3	2.06	0.69
1:A:193:GLU:H	1:A:193:GLU:CD	2.01	0.69
1:B:244:GLN:OE1	4:B:403:HOH:O	2.14	0.65
1:B:1:MET:HE3	1:B:4:LYS:CE	2.29	0.62
1:A:210:ILE:O	1:A:212:PRO:HD3	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:GLU:HB2	1:A:193:GLU:OE2	2.06	0.54
1:B:1:MET:HE3	1:B:4:LYS:HE2	1.90	0.53
1:A:193:GLU:CD	1:A:193:GLU:N	2.66	0.53
1:B:1:MET:HE3	1:B:4:LYS:HE3	1.91	0.52
1:A:164:ILE:CD1	4:A:513:HOH:O	2.59	0.50
1:B:5:HIS:HD2	1:B:99:LYS:NZ	2.13	0.47
1:A:137:HIS:HE1	4:A:404:HOH:O	1.97	0.47
1:A:227:LYS:HE3	1:A:229:TYR:CZ	2.51	0.46
1:B:204:MET:CE	1:B:213[B]:CYS:SG	3.04	0.46
1:A:164:ILE:HD11	4:A:415:HOH:O	2.15	0.45
1:B:164:ILE:HD11	4:B:409:HOH:O	2.16	0.45
1:A:47[B]:ARG:CB	1:A:47[B]:ARG:NH2	2.46	0.45
1:B:99:LYS:HB2	1:B:99:LYS:HE2	1.57	0.45
1:A:112:THR:O	1:A:189:LYS:HE3	2.17	0.44
1:B:164:ILE:CD1	4:B:499:HOH:O	2.66	0.44
1:B:104:LEU:O	1:B:105:ASN:C	2.63	0.42
1:A:41:ALA:HA	1:A:47[B]:ARG:O	2.19	0.41
1:A:215:PHE:CE2	1:A:219:MET:HE2	2.56	0.41
1:B:245:LYS:HD3	1:B:245:LYS:HA	1.97	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	262/260 (101%)	259 (99%)	3 (1%)	0	100	100
1	B	264/260 (102%)	260 (98%)	4 (2%)	0	100	100
All	All	526/520 (101%)	519 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	231/227 (102%)	221 (96%)	10 (4%)	26 4
1	B	233/227 (103%)	230 (99%)	3 (1%)	61 34
All	All	464/454 (102%)	451 (97%)	13 (3%)	39 10

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	3	ARG
1	A	38	GLU
1	A	63	ILE
1	A	71	GLU
1	A	115	PRO
1	A	133[A]	GLU
1	A	133[B]	GLU
1	A	193	GLU
1	A	258	MET
1	B	1	MET
1	B	2	GLU
1	B	92	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	GLN
1	A	224	ASN
1	B	5	HIS
1	B	137	HIS
1	B	141	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	A	301	-	5,5,5	1.29	1 (20%)	5,5,5	0.63	0
2	GOL	A	302	-	5,5,5	0.48	0	5,5,5	0.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	301	-	-	0/4/4/4	-
2	GOL	A	302	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	GOL	O1-C1	2.28	1.52	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	302	GOL	O1-C1-C2-O2
2	A	302	GOL	O1-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	52:VAL	C	53:GLU	N	1.20

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	259/260 (99%)	0.06	6 (2%) 61 67	7, 23, 42, 97	5 (1%)
1	B	259/260 (99%)	-0.11	6 (2%) 61 67	7, 20, 41, 78	7 (2%)
All	All	518/520 (99%)	-0.02	12 (2%) 61 67	7, 21, 41, 97	12 (2%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	259	GLY	4.5
1	B	259	GLY	4.0
1	B	126	PHE	3.8
1	A	258	MET	3.6
1	B	258	MET	3.6
1	B	257	TYR	3.5
1	A	257	TYR	2.8
1	B	1	MET	2.7
1	A	213	CYS	2.4
1	A	1	MET	2.1
1	B	3	ARG	2.0
1	A	46	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

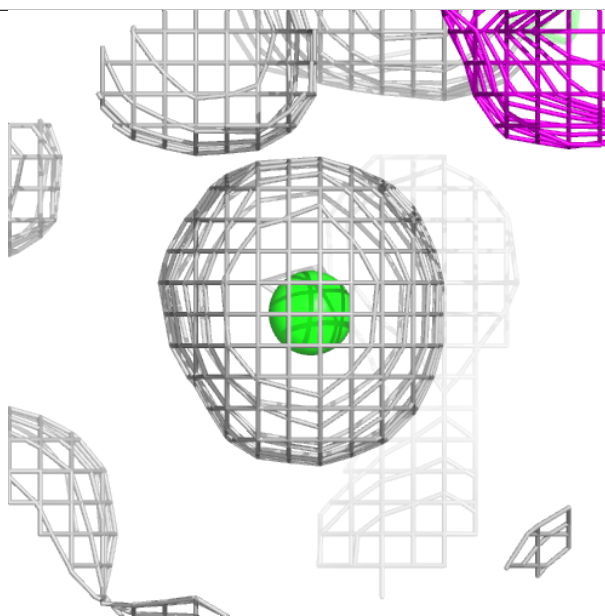
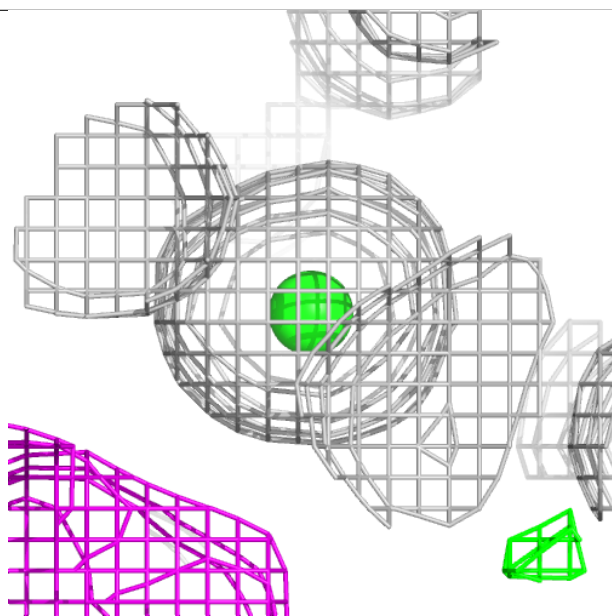
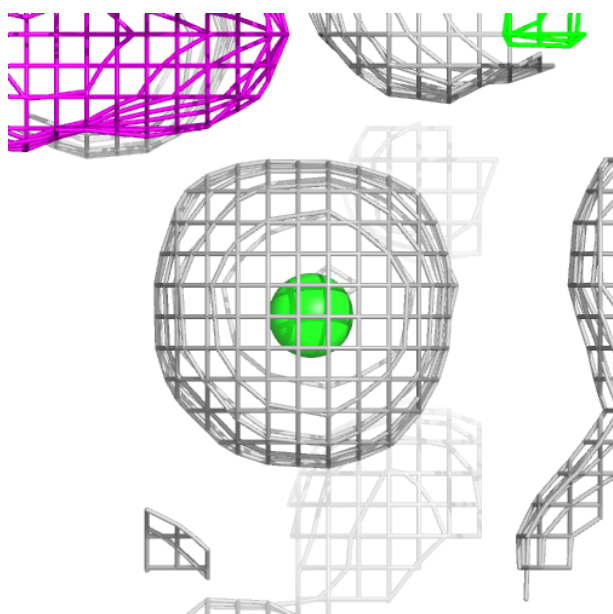
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

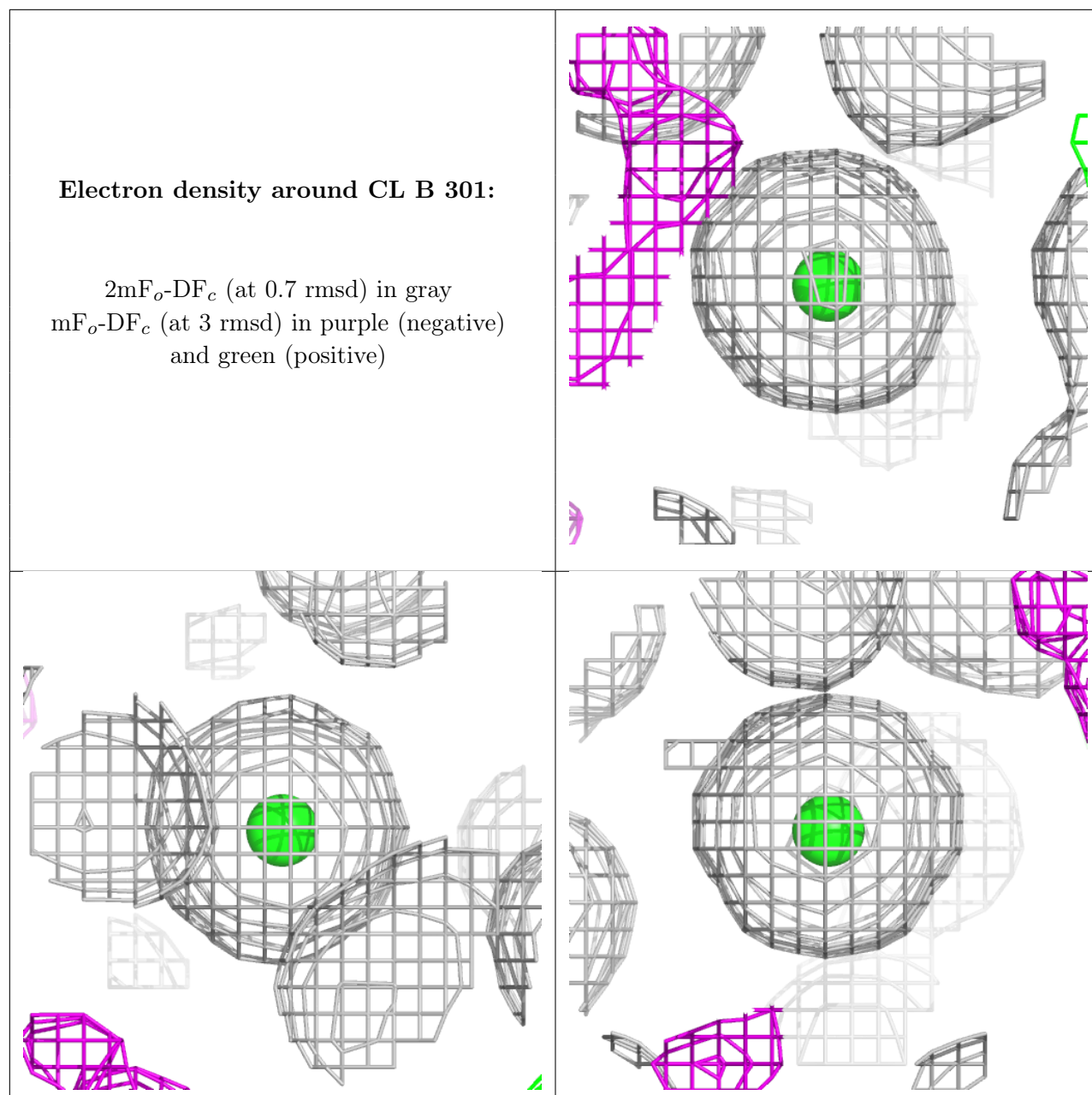
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	A	302	6/6	0.77	0.16	38,44,49,52	0
2	GOL	A	301	6/6	0.94	0.08	23,29,31,38	0
3	CL	A	303	1/1	0.99	0.04	18,18,18,18	0
3	CL	B	301	1/1	1.00	0.03	17,17,17,17	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CL A 303:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.